H20 PHASE CHARACTERIZATION AND ICING MITIGATION THROUGH QUANTUM SENSING IN SILICON CARBIDE NON-METAL DEFECTS

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The primary focus of aircraft icing research has been on ice accretion on wings for its serious adverse consequences. When icing occurs on a wing, the change in airfoil shape results in a decrease in lift and an increase in drag, leading to potentially fatal accidents. Although the issue was recognized in the 1920s, the icing problem is still an area of ongoing research due to the complexity of the icing phenomena [4]. A much-improved understanding of how certain weather conditions produce different icing characteristics will lead to new mitigation methods and a better quantification of current methods. This can be done by better understanding of the molecular bonding energy produced by ice polytype combinations when interacting with different surface materials in various environments [5].

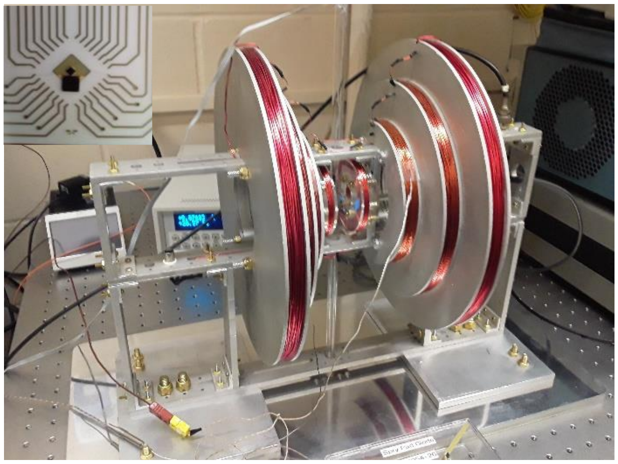
This work is currently developing both models that more accurately describe the quantum signatures of H_2O states (i.e. supercooled, ice, liquid, glass phase...) and chip-based detectors to evaluate these signatures. These sensors utilize ion defects in Silicon Carbide (SiC) as extremely sensitive atomic magnetic detectors. This effort leverages both the decades-long SiC development expertise and infrastructure at NASA Glenn and its growing capabilities in quantum metrology.

Experimental Effort

NV-based magnetometers can detect magnetic fields by optical detection of magnetic resonance (ODMR) or photocurrent detection of magnetic resonance (PDMR) The latter detection technique only requires optical laser excitation and fabrication of electrodes on the diamond chip by standard lithography and avoids the complexity of both optical laser excitation and detection, allowing further miniaturization of the magnetometer. By using this technique, the diamond sensor serves as its own detector [6].

Even though NV Centers in diamond are well-behaved at room temperature and have excellent sensitivity, producing synthetic diamond for quantum devices is still very expensive and integration into circuitry has proven extremely difficult
Instead of synthetic diamond with color impurities, we use SiC (also a large bandgap material) with non-metallic defects (N, F, H, P…) Connect electrodes to the SiC diode. Place the SiC diode in contact with water. The magnetic fields in the water alter the spin states in the defect centers – which effects the output voltage from the SiC diode. Characterize this change in output current for a known phase change in water in contact with the SiC diode. a

High-field and low-field measurement magnetic resonance measurements were accomplished to compare the performance of each non-metal implantation (P-SiC, S-SiC,) in the SiC chip diodes via electrically detectable magnetic resonance (EDMR) e.g., a technique which measures spin dependent electron flow in the presence of a magnetic field. Measurement was promising measuring in the 100's of $nT/\sqrt{Hz}$. Goal is to meet or exceed previous literature values in the 10's of $nT/\sqrt{Hz}$ [7]. Several other non-metal SiC devices were created in the work (H-SiC, B-SiC, N-SiC, O-SiC, F-SiC Cl-SiC) and will be evaluated for their sensitivity. Each device's sensitivity is being gauged to evaluate the possible sensitivities needed to measure hyperfine interactions that are created between the protons of various ice polytypes and the non-metal defects when cycled in and out of resonance. To achieve plan this using electron nuclear double resonance (ENDOR) which combines electronic paramagnetic resonance (EPR) with nuclear magnetic resonance (NMR) to provide a powerful analytical tool that details atomic information and characteristics of nuclei responsible for observed hyperfine splitting. This will be combined with computational efforts to evaluate the environment of those nuclei (H-protons) and thus identify the ice polytype. Figure 1A shows how the magnetic field and RF signal needed for resonance is delivered and Figure 1B shows how they will be used in sensor network for icing mitigation.



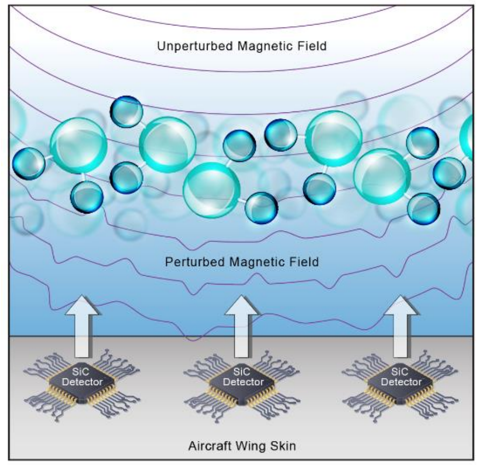


Figure 1 A. RF and Helmholtz coil (inset is SiC device), **B.** Graphic of SiC sensor network on aircraft for icing mitigation

Computational Effort

Ab-initio molecular dynamics (AIMD) simulation of water to compute the infrared spectrum of water was performed. Experiment [1,2] is the condensed phase spectrum of water – which serves as the standard for comparison with our calculation. AIMD is performed on a gas phase, a single, water molecule – employing PBE0/cc-pVTZ model [Figure 2]. Water has three degrees of vibrational freedom, anti-symmetric and symmetric stretch, and scissoring bending. In the bulk phase, the stretching vibrations occur around 3600-3700 cm^{-1} and the bending shows up ~1600 cm^{-1}. In the gas phase, there is a single base peak around 1600 cm^{-1} that exactly matches the bending seen experimentally.

The stretching vibrations, however, show up as one peak and the peak intensity is weak. This could be attributed to two reasons: the first is AIMD simulation employs a single water molecule – which tends to exaggerate quantum effects and observably deviates from the bulk phase generated spectra. The other reason is AIMD usage of basis set and functional. The basis set employed does not fully describe the water system but this remedied could be by systematically making the basis set bigger. The functional, however, can not be systematically improved and it is dependent on the system being simulated. The PBE0 functional is hybrid functional it has been shown to be an improvement over pure DFT and Hartree-Fock exchange functionals [3]. A better approach to this issue is to use a range-separated hybrid DFT functionals that are tuned specifically for the system.

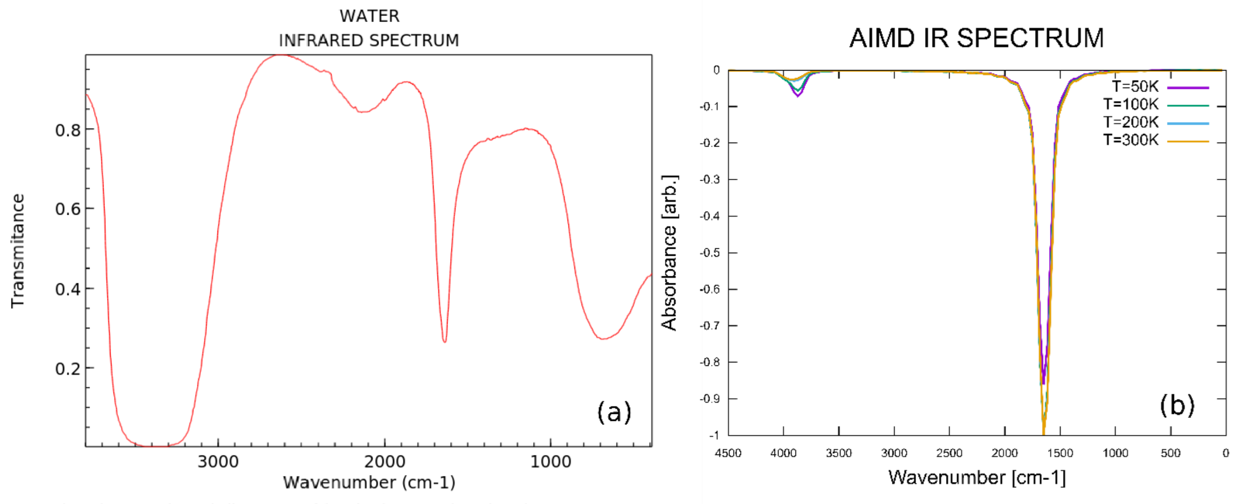


Figure 2 A. Infrared spectrum of water from NIST database [1], **B.** Ab-initio molecular dynamics (AIMD) simulation of water

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